Preprint
UCRL-JC-139517

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This article was submitted to the Materials Research Society 2000 Fall Meeting Conference Proceedings, Boston, Massachusetts, November 27, 2000-December 1, 2001

January 9, 2001

U.S. Department of Energy

Lawrence
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This work was performed under the auspices of the United States Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

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ABSTRACT

Plastic deformation in bcc metals at low temperatures and high-strain rates is controlled by the motion of $a/2\langle 111\rangle$ screw dislocations, and understanding the fundamental atomistic processes of this motion is essential to develop predictive multiscale models of crystal plasticity. The multiscale modeling approach presented here for bcc Ta is based on information passing, where results of simulations at the atomic scale are used in simulations of plastic deformation at mesoscopic length scales via dislocation dynamics (DD). The relevant core properties of $a/2\langle 111\rangle$ screw dislocations in Ta have been obtained using quantum-based interatomic potentials derived from model generalized pseudopotential theory and an *ab-initio* data base together with an accurate Green's-function simulation method that implements flexible boundary conditions. In particular, the stress-dependent activation enthalpy for the lowest-energy kink-pair mechanism has been calculated and fitted to a revealing analytic form. This is the critical quantity determining dislocation mobility in the DD simulations, and the present activation enthalpy is found to be in good agreement with the previous empirical form used to explain the temperature dependence of the yield stress.

INTRODUCTION

The low-temperature and high-strain-rate plastic deformation properties of bcc metals are controlled by $a/2\langle 111\rangle$ screw-dislocation behavior in the crystalline lattice. In particular, the motion of the screw dislocation is believed to be associated with the formation of mobile kinks on the screw dislocation line. Thus, the accurate prediction of kink-pair activation energetics is essential to the understanding and determination of the mobility of screw dislocations in these materials. In turn, an atomistic-based dislocation mobility model is a key ingredient needed to develop predictive multiscale simulations of crystal plasticity for bcc metals.

At higher length scales, the dislocation dynamics (DD) simulation approach has shown some predictive power of the macroscopic plastic response of bcc single crystals based on the fundamental mechanisms of dislocation behavior [1]. However, the accuracy of DD simulations is limited in part by our understanding of the unit dislocation mechanisms and in part by the local rules that dominate the DD simulation process. Therefore, validating a realistic atomistic mobility model is an important first step in developing predictive DD simulations that intend to use atomistic data generated by the proposed kink-pair mechanism. The objectives of this study are twofold. First, it provides a critical link to allow data generated at the atomic length scale to be used directly in mesoscale DD simulations. Second, the DD simulation results can in turn provide a direct comparison with experiment, which is essential to the validation of the atomistic modeling.

In this paper, we report a systematic study of atomistic kink-pair modeling in Ta under an applied shear stress up to $0.4\tau_P$, where τ_P is the calculated Peierls stress to move the straight screw dislocation. Two distinct atomistic approaches were applied to calculate the kink-pair activation enthalpy as a function of applied stress. The results were then fitted to an analytic form that can be directly used as input into the DD simulations. The fitted activation enthalpy obtained from the present atomistic calculations shows good agreement with that previously obtained empirically and used to simulate the observed temperature dependence of the yield stress in Ta [1].

COMPUTATIONAL METHODS

MGPT interatomic potentials

The present calculations in Ta have been carried out using quantum-based, multi-ion interatomic potentials derived from model generalized pseudopotential theory (MGPT) [2]. This approach is based on the corresponding first-principles generalized pseudopotential theory (GPT) [3], which provides a rigorous real-space expansion of the total energy for a bulk transition metal in the form

$$E_{tot}(R_1 \ldots R_N) = NE_{vol}(\Omega) + \frac{1}{2}{\sum_{i,j}}' v_2(ij;\Omega) + \frac{1}{6}{\sum_{i,j,k}}' v_3(ijk;\Omega) + \frac{1}{24}{\sum_{i,j,k,l}}' v_4(ijkl;\Omega) \ , \qquad (1)$$

where $\boldsymbol{R}_1 \ldots \boldsymbol{R}_N$ denote the positions on the N ions in the metal, Ω is the atomic volume, and the prime on each sum over ion positions excludes all self-interaction terms where two indices are equal. The leading volume term in this expansion, E_{vol}, as well as the two-, three-, and four-ion interatomic potentials, v_2, v_3, and v_4, are volume-dependent, but structure-independent quantities and thus transferable to all bulk ion configurations. The angular-force, multi-ion potentials v_3 and v_4 reflect contributions from partially-filled d bands and are generally important for central transition metals. Within the MGPT framework [3], these potentials are systematically approximated by introducing canonical d bands and other simplifications to achieve short-ranged, analytic forms, which can then be applied to both static and dynamic simulations with the Green's function techniques described below. To compensate for the approximations introduced into the MGPT, a limited amount of parameterization is allowed in which the coefficients of the modeled potential contributions are constrained by experimental or volume-dependent *ab-initio* theoretical data. The details of this parameterization for Ta, together with extensive validation tests of the potentials, are discussed in Ref. 4.

Green's function simulation method

In the present work, a method for dynamically updating the boundary conditions of atomistic simulations [5] has been applied to the kink and kink-pair calculations. This approach extends the 2D lattice Green's function (GF) boundary relaxation method originated by Sinclair et al. [6] to 3D simulations, including kink and kink-pair formation. The boundary conditions for 2D and 3D defect cells are evaluated using line [7] and point [8] force distributions, respectively. In this flexible boundary condition method, the simulation box is divided into three regions: atomistic,

GF, and continuum. In the continuum region, the atomistic positions are initially determined according to the anisotropic elastic displacement field [7] for a dislocation line defect at the center of the atomistic region. Complete atomistic relaxation is performed in the atomistic region according to the interatomic forces generated from Eq. (1). Forces develop in the GF region as relaxation is achieved in the atomistic region are then used to relax atoms in all three regions by the 2D or 3D lattice and elastic GF solutions for line [5,7] or point [5,8] forces. The atomistic and GF relaxation are iterated until all force components on each atom are sufficiently small ($< 10^{-4}$ *eV/Å*).

3D dislocation dynamics simulations

The 3D dislocation dynamics simulations are based on a screw-edge description [1], where the dislocation lines are represented by piece-wise connected edge and screw segments. The slip planes are {110} and the Schmid law is assumed to be valid. The unit screw and edge segments are defined as the smallest vectors in <111> and <112> directions, respectively, in a {110} plane and in a simple cubic lattice with a lattice parameter of *2.43 nm*. Isotropic elasticity is used to calculate the internal elastic interactions between the segments. Dislocation mobilities for the edge and the screw are input to the simulation and are defined using so-called 'local rules' [1,9]. In particular, the screw dislocations move by thermally activated kink pair mechanism, and the velocity takes the form [1]:

$$v = b\frac{L}{l_c}(\nu_D \frac{b}{l_c})\exp(-\frac{\Delta H(\tau)}{k_B T}), \quad (2)$$

where b is the magnitude of the Burgers vector, ν_D the Debye frequency, L the screw dislocation length, l_c the critical activation length of a kink pair, and $\Delta H(\tau)$ is the activation enthalpy under local resolved shear stress τ. The edge dislocation mobilities are significantly higher than those of screws [10] and the edges are assumed to move infinitely fast and only stop at their equilibrium lattice positions or when meeting another dislocation line.

The activation enthalpy $\Delta H(\tau)$ was previously extracted from experimental data [1]. It was fitted in the form

$$\Delta H = \Delta H(0)\,[1-(\tau/\tau_P)^p]^q \quad (3)$$

proposed by Kocks, Argon and Ashby [10] with parameters $\Delta H(0)=1.08eV$, $p=0.75$, $q=1.17$, and $\tau_P= 248\ MPa$. The critical activation kink-pair length l_c is taken as $15b$. This set of input to the DD simulations has allowed us to perform simulations at different temperatures and obtained yield stresses as a function of temperature that agree reasonably well with experimental data [1].

RESULTS AND DISCUSSIONS

The unstressed screw dislocation core is predicted to be doubly degenerate and weakly polarized, leading to multiple possible kink pairs involving positive-(*p*) and negative-(*n*) polarized segments [4]. In the low stress limit, when the kink separation is very large (> *20b*), the lowest-energy configuration is found to be *plnnrn* [4,11]. This kink pair has a calculated formation energy of *0.96eV*, which is in close agreement with the empirical zero-stress activation enthalpy obtained in Eq. (3).

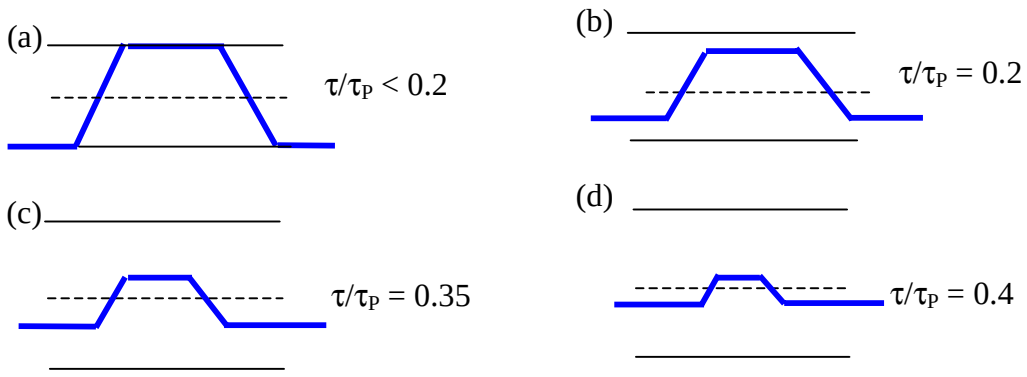

Figure 1. *Schematic drawings of atomistic kink-pair models at different levels of applied shear stress (τ) At low stress levels (τ/τ_P < 0.2), three straight dislocation arms that form the kink-pair are located at the bottom of valley, while at higher stress levels (τ/τ_P > 0.2) the three arms form a metastable configuration that is balanced by the applied shear stress.*

At finite separation, the left and right kinks will elastically attract each other yielding an interaction energy in addition to the zero-stress formation energy. If the kink-kink separation λ is larger than the kink width (~ *7b* for bcc Ta) [4] and the kink height ($h = 2\sqrt{3}b/3$), the total formation energy E_{tot} of a kink pair can then be calculated by summing over the atom-to-atom energy difference between the final equilibrium configuration and a reference configuration, which is a linear combination of unit dislocation disks with *p* or *n* symmetry [4]. In addition, during the kink pair activation process, the energy required to generate the kink pair is supplied partly by thermal activation and partly by the work done by the applied shear stress τ ({110}/<111> in this case) needed to maintain the pair at separation distance λ. The activation enthalpy for such a balanced kink pair is given by

$$\Delta H = E_{tot} - \lambda b h \tau. \quad (4)$$

To investigate the relationships between E_{tot}, and λ and the applied stress τ, we have performed atomistic simulations of a kink-pair under an applied shear stress in a cylinder with the radius of *15b* (for the atomistic region) and the length of *120b*. For very large separations, the formation energy approaches the zero-stress value of *0.96eV* asymptotically. At small separations, the energy decreases rapidly and the stress required to stabilize the kink pair increases sharply. When the separation λ is smaller than the kink width, which corresponds to an applied shear stress $\tau > 0.2\tau_P$, the assumption of weakly interacting kinks in our atomistic simulations is breaking down in this regime [4]. This may be attributed to the fact that the assumed dislocation configuration is in an unstable equilibrium state. At higher stress levels, a self-consistent 3D atomistic model of kink-pair formation and migration is therefore necessary (Fig. 1) [12]. Here we report simulation results up to an applied shear stress level of $0.4\tau_P$. To calculate the kink-pair formation enthalpy under such an applied shear stress, three new steps are taken in our 3D atomistic simulations: (1) A straight *a*/2<111> screw dislocation is constructed and is then fully relaxed under a pre-defined applied stress. This procedure provides the necessary building block for the 3D kink-pair model that will be constructed in step (2). As a result, the straight screw dislocation line is lifted above the valley of the Peierls potential, and the degree of lifting depends on the magnitude of the applied shear stress. (2) A 3D atomistic kink-

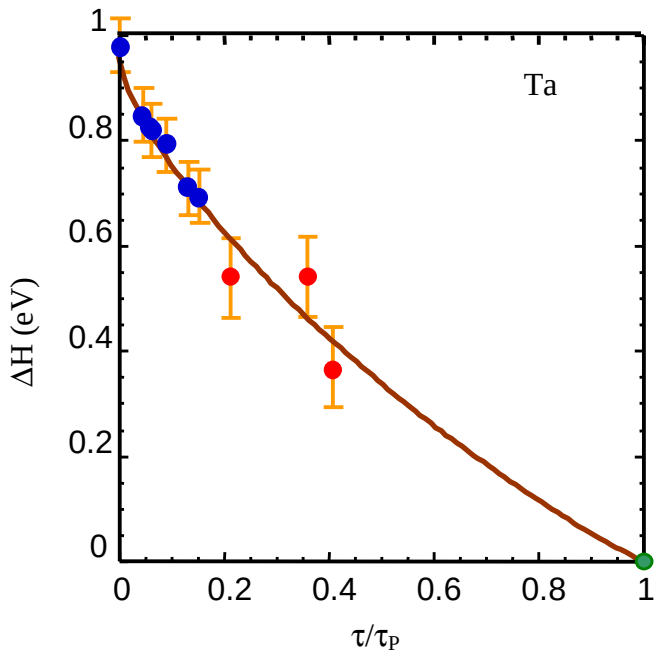

Figure 2. *Activation enthalpy (ΔH) as a function of applied stress (τ/τ_P) for bcc Ta. Here two different atomistic kink-pair models are used for these calculations, depending on whether $\tau/\tau_P < 0.2$ or > 0.2 (Fig. 1). The solid line is a fit to the calculated results in the form of Eq. (3) and the error bars indicate the numerical uncertainty in our atomistic simulations.*

pair model is constructed according the reference configuration generated from step (1). Under this construction, the separation λ is treated as a fixed parameter during the atomistic energy minimization. The total energy (E_{tot}) is then calculated by summing over the atom-to-atom energy difference between the fully relaxed 3D configuration and the fundamental straight screw dislocation under the pre-defined applied shear stress. (3) Finally, the work done by the applied stress is then estimated using a trapezoid model [13] and the response stress due to the kink-pair formation at the separation λ. The calculated activation enthalpy is displayed in Fig. 2. This result shows great improvement over using the low-stress kink-pair model at stresses $\tau/\tau_P > 0.2$, as in Ref. [4], where the kink pair was constructed from a relaxed straight dislocation at zero stress [Fig. 1(a)].

The new data was then fitted to Eq. (2) for the kink-pair activation enthalpy. In this fit we used $\Delta H(0)=0.96eV$, the kink-pair formation energy at zero stress, and $\tau_P=606MPa$, the calculated Peierls stress in {110} plane. Our calculated τ_P is actually about 2 times larger than the best available experimental estimate (*248 MPa*) for bcc Ta [14], and the possible reasons for this discrepancy are discussed in Ref. 4. This is an issue for further study. However, when fitting to the scaled stress value τ/τ_P, the fitted parameters $p=0.71$ and $q=1.10$ agree quite well with the parameters obtained by fitting to experimental data, *0.75* and *1.17*, as indicated above. This good agreement in fact suggests that the proposed atomistic kink-pair mechanisms under applied stress levels up to $0.4\tau_P$ correctly reflect the actual screw dislocation processes at low temperatures.

SUMMARY

In summary, we have reported a systematic study of atomistic kink-pair modeling in Ta under an applied shear stress up to $0.4\tau_P$. Low- and high-stress atomistic models were used to calculate the kink-pair activation enthalpy as a function of applied shear stress. The results were then fitted to an analytic form that provides critical input into 3D DD simulations. Within the accuracy of our atomistic simulations, the fitted parameters agree well with the ones used in previous DD simulations to accurately calculate the single-crystal yield stress as a function of temperature [1]. In the near future, we plan to apply the present approach over a wide range of pressure- and stress-orientation conditions. This will provide the necessary input into the 3D DD simulations to predict the yield stress in bcc Ta at these conditions.

ACKNOWLEDGMENTS

Many discussions with the late Dr. M. Duesbery and Prof. V. Vitek are greatly appreciated. This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

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